Unstructured Randomness, Small Gaps and Localization

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We study the Hamiltonian associated with the quantum adiabatic algorithm with a random cost function. Because the cost function lacks structure we can prove results about the ground state. We find the ground state energy as the number of bits goes to infinity, show that the minimum gap goes to zero exponentially quickly, and we see a localization transition. We prove that there are no levels approaching the ground state near the end of the evolution. We do not know which features of this model are shared by a quantum adiabatic algorithm applied to random instances of satisfiability since despite being random they do have bit structure.

I. INTRODUCTION, DISCUSSION, AND CONCLUSIONS

Recently there has been interest in the relevance of Anderson localization to the quantum adiabatic algorithm[1, 2, 8]. In this paper we study properties of the Hamiltonian associated with the adiabatic algorithm with a cost function that has random (essentially) uncorrelated values. The cost function we look at does not have the structure present in cost functions produced by random instances of satisfiability. This lack of structure makes our example analyzable and the localization transition and corresponding small gap will be evident. The model is a spin Hamiltonian on n spins that takes the form

$$H(s) = (1-s)\sum_{i=1}^{n}\left(\frac{1-\sigma_x^i}{2}\right) + s\sum_{z=0}^{2^n-1} E(z)|z\rangle\langle z|. \tag{1}$$

The "on site energies" $E(z)$ are random variables obtained by scrambling the Hamming weight cost function. Viewing z in (1) as an n bit string, the Hamming weight $W(z)$ is the number of ones in the string. Let π be a random permutation of the 2^n integers between 0 and 2^n-1. By "random permutation" we mean that all $2^n!$ permutations are equally likely. Note we are permuting the 2^n strings, not the n bits. Then

$$E(z) = W(\pi^{-1}(z)) \tag{2}$$

and

$$H_\pi(s) = (1-s)\sum_{i=1}^{n}\left(\frac{1-\sigma_x^i}{2}\right) + s\sum_{z=0}^{2^n-1} W(\pi^{-1}(z))|z\rangle\langle z|. \tag{3}$$

In figure 1 we plot the lowest 25 energy levels of this Hamiltonian, as a function of s, with $n = 18$ and with a particular random choice of the permutation π. Different random permutations produce very similar pictures. The ground state energy is well approximated by two straight lines[5, 7, 10]. We will prove that asymptotically (in n) they are in fact straight lines. At $s = \frac{1}{2}$ the gap between the ground state and the first excited state is small and we will show that asymptotically the minimum gap is exponentially small in n.

This Hamiltonian is similar to the "random energy model" of the form (1) with on site energies chosen i.i.d, that is, independently and identically distributed. Some of what we prove is already known for the random energy model[7, 10, 11]. For example, in [7], Jörg et. al. use perturbation theory to show the existence of a first order phase transition in a random energy model. In contrast, we use variational methods which prove upper and lower bounds on the ground state energy. To prove that the gap is exponentially small in n, we use the information theoretic result[5] that no efficient quantum algorithm exists for locating the minimum of a scrambled cost function.

It is apparent from the picture that the ground state changes dramatically at $s = \frac{1}{2}$. In fact for $s < \frac{1}{2}$, the ground state is very close to the ground state at $s = 0$,

$$|x = 0\rangle = \frac{1}{\sqrt{2^n}} \sum_{z=0}^{2^n-1} |z\rangle$$

which in the z basis is completely delocalized. For $s > \frac{1}{2}$ the ground state is close to the ground state at $s = 1$ which is

$$|z = \pi(0)\rangle$$

corresponding to one z string, that is, a fully localized state.

The small gap just seen at $s = \frac{1}{2}$ is associated with a "delocalized to localized" first order phase transition. Recently it has been suggested that a "localized to localized" ground state transition can also lead to an exponentially small gap. These ground state transitions, studied in [1–4, 8], can be seen using low order perturbation theory, and occur for $s \to 1$ as $n \to \infty$. There are two key features of a model that exhibits these perturbative crosses. First, for any string a single bit flip changes the cost function by $O(1)$. The other feature is that there are very disparate bit strings with low cost. The scrambled model that we study has the second feature but not the first and we show that perturbative crosses are not present. We prove that for $s \geq 0.9$ the gap is greater than a positive constant independent of n.

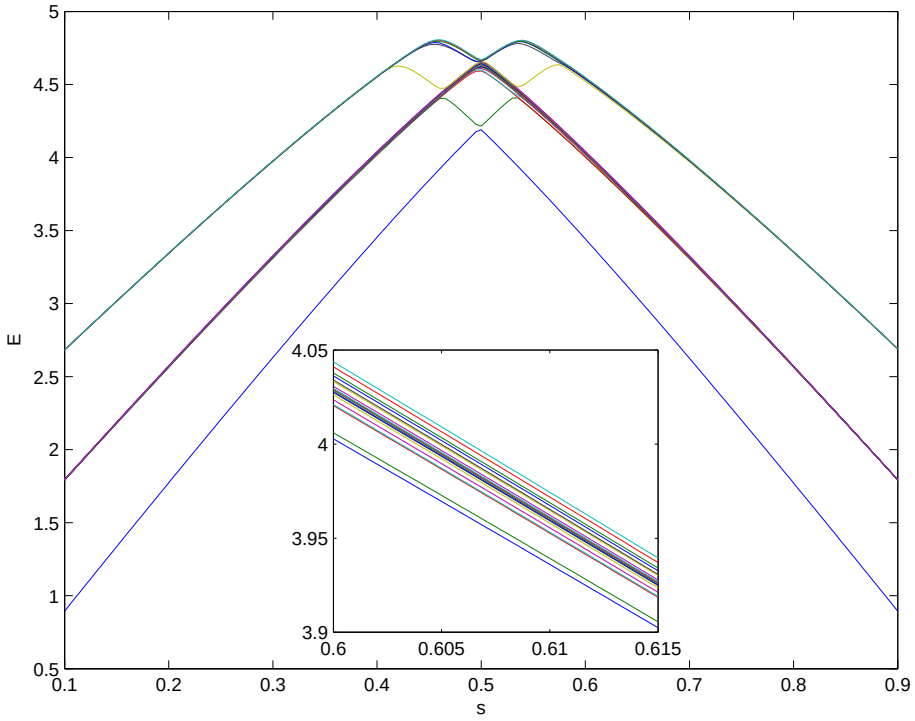

Figure 1: Lowest 25 energy levels for an instance with a random permutation at $n = 18$. The inset shows a magnified view of levels 2 through 19 near $s = 0.6$.

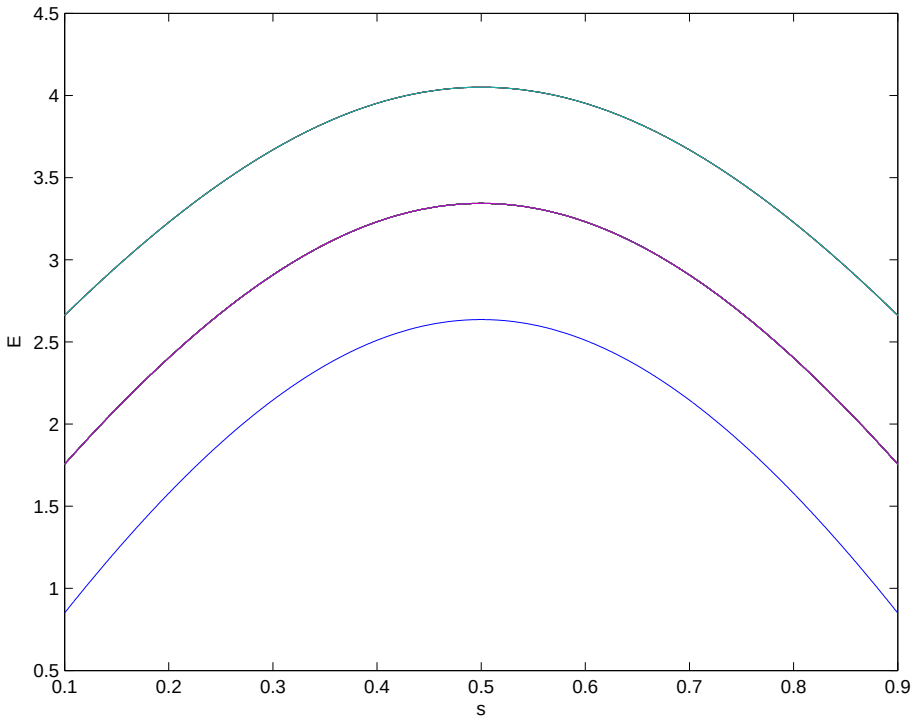

Figure 2: Lowest 25 levels for the instance with the identity permutation at $n = 18$.

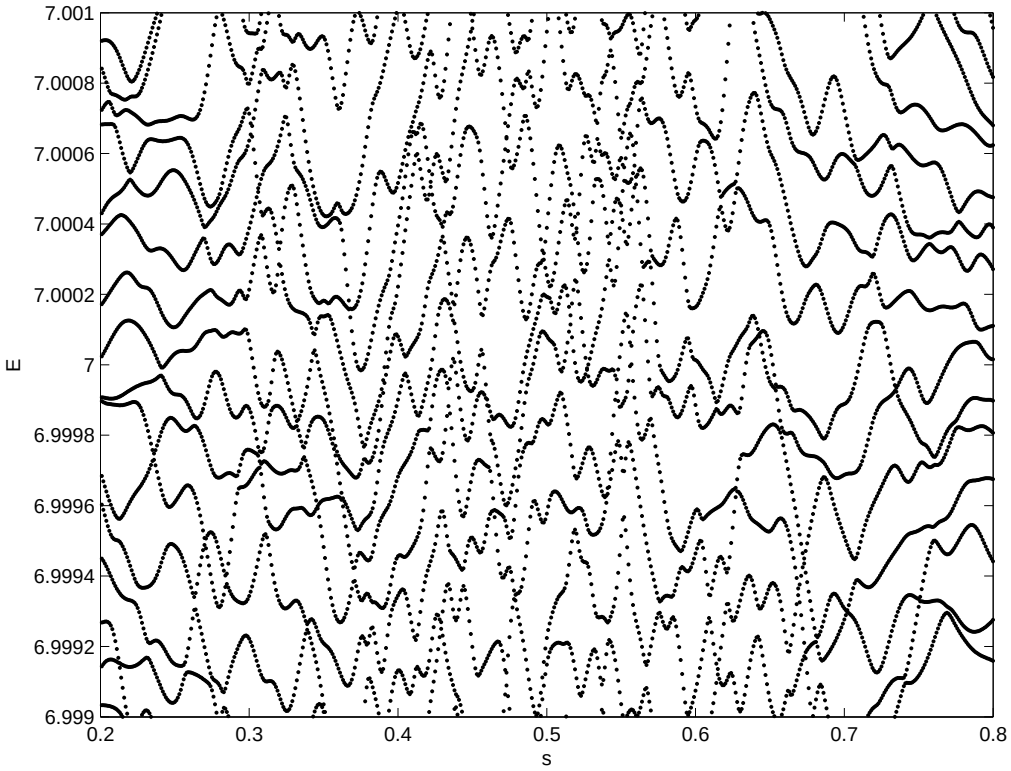

Figure 3: Energy levels in the middle of the spectrum for a 14 spin instance with a random permutation.

The regularity in figure 1 and the simple description of the ground state are consequences of the total lack of structure in the scrambled cost function. Although it is not relevant to the performance of the adiabatic algorithm, it is interesting to look at the middle of the spectrum. In figure 3 we show energy levels in the middle of the spectrum for a random choice of π at $n = 14$. Here there are many avoided crosses and no apparent regularity in contrast to the bottom of the spectrum.

Suppose the permutation π used to generate figure 1 were replaced by the identity. Now the cost function, $E(z) = W(z)$, is the unscrambled Hamming weight and the Hamiltonian (3) is a sum of n one qubit Hamiltonians making it easy to analyze. The lowest 25 levels for $n = 18$ are shown in figure 2. Note that the minimum gap is independent of n. Furthermore the values and degeneracies of the on site energies in figure 2 are the same as those in figure 1. The radical differences between these figures are caused by the bit structure present in the unscrambled case but absent in the scrambled case.

It is not yet known how the quantum adiabatic algorithm performs on random instances of satisfiability, for example, instances of Exact Cover generated by random choices of 3 bits [12, 13]. Despite the randomness, these Hamiltonians still have bit structure. We do not know if random instances of satisfiability have a "delocalized to localized" first order phase transition like the fully

unstructured example shown in figure 1 or have no "delocalized to localized" phase transition like the bit structured example shown in figure 2.

II. RESULTS

For a given n and π we have $H_\pi(s)$ given by (3). Denote the ground state energy by $E_\pi(s)$. Also let

$$e(s) = \begin{cases} \frac{s}{2} & \text{for } 0 \le s \le \frac{1}{2} \\ \frac{(1-s)}{2} & \text{for } \frac{1}{2} \le s \le 1. \end{cases} \tag{4}$$

We have 3 results which suffice for our needs but are not best possible. First $\frac{E_\pi(s)}{n}$ is well approximated by $e(s)$ for n large.

Theorem 1. *Let π be a random permutation. Then*

$$\frac{E_\pi(s)}{n} \le e(s) \text{ for all } 0 \le s \le 1$$

and

$$Pr\left[\frac{E_\pi(s)}{n} \ge e(s)\left[1 - 5n^{-\frac{1}{4}}\right] \text{ for all } 0 \le s \le 1\right] \to 1 \text{ as } n \to \infty.$$

By $Pr\,[event]$ we mean the probability that the *event* occurs where the distribution is over π chosen with equal probability from the $2^n!$ permutations.

Our next result is that the minimum gap is exponentially small in n. For each π let

$$g_\pi = \min_{0 \le s \le 1} \gamma_\pi(s).$$

where $\gamma_\pi(s)$ is the eigenvalue gap between the two lowest energy levels of $H_\pi(s)$.

Theorem 2. *Let π be a random permutation. Then*

$$Pr\left[g_\pi \le n^2 2^{-\frac{n}{6}}\right] \to 1 \text{ as } n \to \infty.$$

Our last result is that typically $\gamma_\pi(s)$ is larger than some n independent constant for s near 1.

Theorem 3. *Let π be a random permutation. Then*

$$Pr[\gamma_\pi(s) > 0.8 \text{ for } .9 \leq s \leq 1] \to 1 \text{ as } n \to \infty.$$

A. A Lower Bound For the Ground State Energy of Stoquastic Hamiltonians

For any normalized state $|\psi\rangle$, and any Hamiltonian H, the quantity $\langle\psi|H|\psi\rangle$ is an upper bound on the ground state energy. It is less well known that, for some special Hamiltonians, one can also obtain a variational lower bound on the ground state energy of H. Theorem 4 (given below) is an example of such a bound. It is an elementary application of the Collatz Wielandt min-max formula [9], but we prove it here for completeness. We restrict to Hamiltonian matrices H where all off diagonal matrix elements are real and nonpositive. These are called stoquastic Hamiltonians (note that stoquasticity is a basis dependent notion).

Theorem 4. *Let H be a Hermitian operator, stoquastic in the $|z\rangle$ basis, that is $\langle z|H|z'\rangle \leq 0$ for $z \neq z'$. Let E_g be its lowest eigenvalue. Then*

$$E_g \geq \min_z \frac{\langle z|H|\phi\rangle}{\langle z|\phi\rangle}$$

for any state $|\phi\rangle$ such that $\langle z|\phi\rangle > 0$ for all z.

The following Lemma will be used in our proof of Theorem 4.

Lemma 1. *Let H be a Hermitian operator, stoquastic in the $|z\rangle$ basis, that is $\langle z|H|z'\rangle \leq 0$ for $z \neq z'$. If $H|\psi\rangle = E|\psi\rangle$ and $\langle z|\psi\rangle > 0$ for all z, then $E = E_g$, the ground state energy of H.*

Proof. Suppose $E > E_g$. Let $|\psi_g\rangle$ be any (normalized) state in the ground state subspace of H, so that $H|\psi_g\rangle = E_g|\psi_g\rangle$. Divide the values of z into 3 sets:

$$\begin{aligned} S_+ &= \{z : \langle z|\psi_g\rangle > 0\} \\ S_- &= \{z : \langle z|\psi_g\rangle < 0\} \\ S_0 &= \{z : \langle z|\psi_g\rangle = 0\}. \end{aligned}$$

Define $|\psi'_g\rangle$ by

$$\langle z|\psi'_g\rangle = |\langle z|\psi_g\rangle|.$$

Then $|\psi_g'\rangle$ is normalized and by the variational principle

$$\langle\psi_g'|H|\psi_g'\rangle - \langle\psi_g|H|\psi_g\rangle \geq 0.$$

But

$$\begin{aligned}\langle\psi_g'|H|\psi_g'\rangle - \langle\psi_g|H|\psi_g\rangle &= -4\sum_{z\in S_+}\sum_{z'\in S_-}\langle z|\psi_g\rangle\langle z'|\psi_g\rangle\langle z|H|z'\rangle \\ &\leq 0\end{aligned}$$

where in the last line we have used the stoquasticity of H. Therefore

$$\langle\psi_g'|H|\psi_g'\rangle = \langle\psi_g|H|\psi_g\rangle = E_g$$

and so $H|\psi_g'\rangle = E_g|\psi_g'\rangle$. This implies $\langle\psi|\psi_g'\rangle = 0$, which is impossible since $|\psi\rangle$ has only positive coefficients in the z basis and $|\psi_g'\rangle$ has nonnegative coefficients. So we have reached a contradiction and therefore $E = E_g$. □

Proof of Theorem 4

Let $\hat{H}$ be

$$\hat{H} = H - \sum_z |z\rangle\langle z|\frac{\langle z|H|\phi\rangle}{\langle z|\phi\rangle}.$$

Note that $|\phi\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue 0. The ground state energy of $\hat{H}$ is 0 by Lemma 1.

For any normalized state $|\psi\rangle$ we have

$$\begin{aligned}\langle\psi|H|\psi\rangle - \langle\psi|\hat{H}|\psi\rangle &= \sum_z |\langle z|\psi\rangle|^2\left[\frac{\langle z|H|\phi\rangle}{\langle z|\phi\rangle}\right] \\ &\geq \min_z\left[\frac{\langle z|H|\phi\rangle}{\langle z|\phi\rangle}\right].\end{aligned}$$

Choosing $|\psi\rangle$ to be a ground state of H we have

$$E_g - \langle\psi|\hat{H}|\psi\rangle \geq \min_z\left[\frac{\langle z|H|\phi\rangle}{\langle z|\phi\rangle}\right].$$

But $\langle\psi|\hat{H}|\psi\rangle \geq 0$ since $\hat{H}$ has ground state energy 0, so

$$E_g \geq \min_z \frac{\langle z|H|\phi\rangle}{\langle z|\phi\rangle}.$$

B. Proof of Theorem 1

First for the upper bound. Recall that

$$|x=0\rangle = \frac{1}{\sqrt{2^n}} \sum_z |z\rangle$$

is the ground state of $H_\pi(0)$. Using this state we get an upper bound on the ground state energy

$$E_\pi(s) \leq \langle x=0|H_\pi(s)|x=0\rangle = s\frac{n}{2}. \tag{5}$$

Recall that $|\pi(0)\rangle$ is the ground state of $H_\pi(1)$. Using this state we get the upper bound

$$E_\pi(s) \leq \langle \pi(0)|H_\pi(s)|\pi(0)\rangle = (1-s)\,\frac{n}{2}$$

for $0 \leq s \leq 1$. These two inequalities establish the upper bound in Theorem 1.

Proving the lower bound is more involved. We first use Theorem 4 to show that with high probability the ground state energy $E_\pi(s^\star)$ at $s^\star$ just above $\frac{1}{2}$ is close to the value $n \cdot e(s^\star)$. Then we use the concavity of $E_\pi(s)$ to obtain the lower bound for all $s \in [0,1]$.

We use an ansatz $|A_\pi\rangle$ for the ground state of $H_\pi(s^\star)$ of the form

$$\langle z|A_\pi\rangle = \begin{cases} 1 & ,\ \mathrm{z} \notin S_\pi \\ \lambda n & ,\ \mathrm{z} \in S_\pi \end{cases} \tag{6}$$

where λ satisfies $\lambda n > 1$ for n large and S_π is a set of low energy bit strings,

$$S_\pi = \left\{ z :\ W(\pi^{-1}(z)) \leq nc \right\}$$

with $c < \frac{1}{2}$. We can view S_π as the image under π of the set of strings with Hamming weight less than nc:

$$\begin{aligned} S_\pi &= \pi(L) \\ L &= \{ z :\ W(z) \leq nc \}. \end{aligned}$$

The following lemma bounds the probability that a group of bit strings related by single bit flips are all in a random set.

Lemma 2. *Let M be a set of n-bit strings such that*

$$|M| \leq 2^{n\gamma}$$

for some $0 < \gamma < 1$. Let k be an integer. Let π be a random permutation of the set of all n-bit strings, and consider $\pi(M)$, the image of the set M. Let p be the probability that there exists an n-bit string z and a set of $k-1$ bits $\{i_1, i_2, ..., i_{k-1}\}$ such that $\left\{z, z \oplus e_{i_1}, ..., z \oplus e_{i_{k-1}}\right\} \subseteq \pi(M)$. Similarly let q be the probability that there exists an n-bit string y and a set of k bits $\{j_1, j_2, ..., j_k\}$ such that $\{y \oplus e_{j_1}, ..., y \oplus e_{j_k}\} \subseteq \pi(M)$. Then

$$p \leq n^k 2^{n[1-k(1-\gamma)]}$$

and

$$q \leq n^k 2^{n[1-k(1-\gamma)]}\,.$$

Proof. Fix a particular z and a set of $k-1$ bits $\{i_1, i_2, ..., i_{k-1}\}$. Then

$$\begin{aligned}\Pr\left[\left\{z, z \oplus e_{i_1}, ..., z \oplus e_{i_{k-1}}\right\} \subseteq \pi(M)\right] &= \frac{|M| \cdot (|M|-1) \ldots (|M|-k+1)}{2^n \cdot (2^n-1) \ldots (2^n-k+1)} \\ &\leq \left(\frac{|M|}{2^n}\right)^k.\end{aligned}$$

There are 2^n choices for z and $\begin{pmatrix} n \\ k-1 \end{pmatrix}$ choices for the set of $k-1$ bits so by a union bound

$$\begin{aligned}p &\leq 2^n \begin{pmatrix} n \\ k-1 \end{pmatrix} \left(\frac{|M|}{2^n}\right)^k \\ &\leq n^k 2^{n[1-k(1-\gamma)]}\,.\end{aligned}$$

The proof for q is very similar. □

Lemma 3. *Let $s^\star = \frac{1}{2} + n^{-\frac{1}{4}}$. Let π be a random permutation. Then*

$$Pr\left[E_\pi(s^\star) \geq \left(\frac{1-s^\star}{2}\right)\left(n - n^{\frac{3}{4}}\right)\right] \to 1 \text{ as } n \to \infty.$$

Proof. Return to S_π and set $c = \frac{1}{2} - \frac{1}{2}n^{-\frac{1}{4}}$. We will show that the state $|A_\pi\rangle$ from (6) (with λ specified later) furnishes the claimed lower bound on the ground state energy when plugged into Theorem 4. In order to do this we establish some properties of the set S_π. First

$$\begin{aligned}|S_\pi| &= \sum_{j=1}^{\lfloor cn \rfloor} \begin{pmatrix} n \\ j \end{pmatrix} \\ &\leq \left(\frac{1}{c^c\,(1-c)^{1-c}}\right)^n.\end{aligned}$$

This upper bound on $|S_\pi|$ follows directly from the Chernoff-Hoeffding bound. Now let

$$f(x) = -x\log_2(x) - (1-x)\log_2(1-x) \tag{7}$$

so

$$\left(\frac{1}{c^c\,(1-c)^{1-c}}\right)^n = 2^{nf(c)}.$$

Now

$$\begin{aligned} f(c) \;&=\; f(\frac{1}{2} - \frac{1}{2}n^{-\frac{1}{4}}) = 1 - \frac{1}{\ln 2}\left[\frac{1}{1\cdot 2}\left(\frac{1}{n}\right)^{\frac{1}{2}} + \frac{1}{3\cdot 4}\left(\frac{1}{n}\right) + \frac{1}{5\cdot 6}\left(\frac{1}{n}\right)^{\frac{3}{2}} + ...\right] \\ &\leq\; 1 - \frac{1}{2\ln 2}\left(\frac{1}{\sqrt{n}}\right), \end{aligned}$$

so $|S_\pi| \leq 2^{n\left(1-\frac{1}{2\ln 2}\left(\frac{1}{\sqrt{n}}\right)\right)}$.

Lemma 2 says that the probability p that a set $\left\{z, z\oplus e_{j_1}, z\oplus e_{j_2}, ..., z\oplus e_{j_{k-1}}\right\} \subseteq S_\pi$ exists satisfies

$$\begin{aligned} p \;&\leq n^k \;\; 2^{n\left[1-\frac{k}{2\ln 2}\left(\frac{1}{\sqrt{n}}\right)\right]} \\ &=\quad 2^{\left[k\frac{\ln n}{\ln 2} + n - \frac{k\sqrt{n}}{2\ln 2}\right]}. \end{aligned}$$

We now choose

$$k = \lceil\, 2\sqrt{n}\,\rceil$$

so that this probability goes to 0 as $n\to\infty$. With high probability there is no set consisting of more than $k-2$ one bit flip neighbors of z in S_π when z is in S_π. So

$$\Pr\left[\sum_{i=1}^{n}\frac{\langle z\oplus e_i|A_\pi\rangle}{\langle z|A_\pi\rangle} \leq \frac{[\lambda n\,(k-2) + 1\cdot(n-k+2)]}{\lambda n} \text{ for all } z\in S_\pi\right] \to 1 \text{ as } n\to\infty.$$

Similarly the probability that a set of the form $\{z\oplus e_{i_1}, z\oplus e_{i_2}, ..., z\oplus e_{i_k}\} \subseteq S_\pi$ exists goes to zero as $n\to\infty$. That is, with high probability there is no set consisting of more than $k-1$ one bit flip neighbors of z in S_π for $z\notin S_\pi$. So

$$\Pr\left[\sum_{i=1}^{n}\frac{\langle z\oplus e_i|A_\pi\rangle}{\langle z|A_\pi\rangle} \leq \lambda n\,(k-1) + 1\cdot(n-k+1) \text{ for all } z\notin S_\pi\right] \to 1 \text{ as } n\to\infty.$$

Let us compute the lower bound on the ground state energy $E_g(s^\star)$ that is obtained by using $|A_\pi\rangle$ in Theorem 4 assuming both of these events occur. We get

$$\begin{aligned}\frac{\langle z|H_\pi(s^\star)|A_\pi\rangle}{\langle z|A_\pi\rangle} &= s^\star E(z) + \left(\frac{1-s^\star}{2}\right)n - \left(\frac{1-s^\star}{2}\right)\sum_{i=1}^{n}\frac{\langle z\oplus e_i|A_\pi\rangle}{\langle z|A_\pi\rangle} \\ &\geq \begin{cases} \left(\frac{1-s^\star}{2}\right)n - \left(\frac{1-s^\star}{2}\right)\left[\frac{\lambda n\,(k-2)+1\cdot(n-k+2)}{\lambda n}\right] & ,\text{ for } z\in S_\pi \\ s^\star\cdot nc + \left(\frac{1-s^\star}{2}\right)n - \left(\frac{1-s^\star}{2}\right)\left[\lambda n\,(k-1)+1\cdot(n-k+1)\right] & ,\text{ for } z\notin S_\pi\,. \end{cases}\end{aligned}$$

Now choose

$$\lambda = \frac{1}{k-1}\left(\frac{2s^\star c}{1-s^\star} - 1\right)$$

so

$$\begin{aligned}\frac{\langle z|H_\pi(s^\star)|A_\pi\rangle}{\langle z|A_\pi\rangle} &\geq \begin{cases} \left(\frac{1-s^\star}{2}\right)n - \left(\frac{1-s^\star}{2}\right)\left[\frac{\lambda n\,(k-2)+1\cdot(n-k+2)}{\lambda n}\right] & ,\text{ for } z\in S_\pi \\ \left(\frac{1-s^\star}{2}\right)n + \left(\frac{1-s^\star}{2}\right)(k-1) & ,\text{ for } z\notin S_\pi \end{cases} \\ &\geq \left(\frac{1-s^\star}{2}\right)\left[n-(k-2)-\frac{1}{\lambda}\right] \text{ for all } z.\end{aligned}$$

Recall that we picked $c = \frac{1}{2} - \frac{1}{2}n^{-\frac{1}{4}}$ and $s^\star = \frac{1}{2} + n^{-\frac{1}{4}}$. This gives

$$\lambda = \frac{1}{k-1}\left(3\left(\frac{1}{n^{\frac{1}{4}}}\right) + 4\left(\frac{1}{n^{\frac{1}{4}}}\right)^2 + 8\left(\frac{1}{n^{\frac{1}{4}}}\right)^3 + ...\right)$$

which means, since $k = \lceil\, 2\sqrt{n}\,\rceil$, that $\lambda \geq \frac{3}{2}n^{-\frac{3}{4}}$ and

$$\frac{\langle z|H_\pi(s^\star)|A_\pi\rangle}{\langle z|A_\pi\rangle} \geq \left(\frac{1-s^\star}{2}\right)\left[n - n^{\frac{3}{4}}\right] \text{ for all } z$$

with probability approaching 1 as $n\to\infty$. Applying Theorem 4 completes the proof of Lemma 3. □

We are now ready to prove the lower bound on $E_\pi(s)$ which is claimed in Theorem 1. Since $H_\pi(s)$ is linear in s we can write

$$H_\pi(s) = \left(\frac{s-s_1}{s_2-s_1}\right)H_\pi(s_2) + \left(\frac{s_2-s}{s_2-s_1}\right)H_\pi(s_1)$$

and taking the expectation of both sides in the ground state of $H_\pi(s)$ gives, for $s_1 < s < s_2$,

$$E_\pi(s) \geq \left(\frac{s-s_1}{s_2-s_1}\right)E_\pi(s_2) + \left(\frac{s_2-s}{s_2-s_1}\right)E_\pi(s_1) \tag{8}$$

by the variational principle. Since $E_\pi(0) = 0$ this gives

$$E_\pi(s) \geq \frac{s}{s^\star} E_\pi(s^\star).$$

Using Lemma (3) we get that with probability $\to 1$ as $n \to \infty$

$$E_\pi(s) \geq \frac{s}{s^\star}\left(\frac{1-s^\star}{2}\right)\left[n - n^{\frac{3}{4}}\right] \quad \text{for } 0 \leq s \leq s^\star$$

and recalling that $s^\star = \frac{1}{2} + n^{-\frac{1}{4}}$ gives

$$\begin{aligned} E_\pi\left(\tfrac{1}{2}\right) &\geq \frac{n}{4}\left(\frac{\frac{1}{2} - n^{-\frac{1}{4}}}{\frac{1}{2} + n^{-\frac{1}{4}}}\right)\left(1 - n^{-\frac{1}{4}}\right) \\ &\geq \frac{n}{4}\left(1 - 5n^{-\frac{1}{4}}\right). \end{aligned}$$

Using (8) again twice (with $s_1 = 0$, $s_2 = \frac{1}{2}$ and with $s_1 = \frac{1}{2}$, $s_2 = 1$) we get

$$\frac{E_\pi(s)}{n} \geq e(s)\left[1 - 5n^{-\frac{1}{4}}\right]$$

for $0 \leq s \leq 1$ with probability $\to 1$ as $n \to \infty$, which completes the proof.

C. Proof of Theorem 2

We will use the adiabatic theorem (in the form given in Theorem 3 of [6] with $m = 1$) as well as a theorem from [5]. For completeness we reproduce the statements of these theorems here:

Adiabatic Theorem (from [6]). *Let $H(s)$ be a finite-dimensional twice differentiable Hamiltonian on $0 \leq s \leq 1$ with a nondegenerate ground state $|\phi(s)\rangle$ separated by an energy gap $\gamma(s)$. Let $|\psi(t)\rangle$ be the state obtained by Schrödinger time evolution with Hamiltonian $H\left(\frac{t}{T}\right)$ starting with state $|\phi(0)\rangle$ at $t = 0$. Then*

$$\sqrt{1 - |\langle\psi(T)|\phi(1)\rangle|^2} \leq \frac{1}{T}\left[\frac{1}{\gamma(0)^2}\left\|\frac{dH}{ds}\right\|_{s=0} + \frac{1}{\gamma(1)^2}\left\|\frac{dH}{ds}\right\|_{s=1} + \int_0^1 ds\left(\frac{7}{\gamma^3}\left\|\frac{dH}{ds}\right\|^2 + \frac{1}{\gamma^2}\left\|\frac{d^2H}{ds^2}\right\|\right)\right].$$

The next theorem considers the complexity of finding the minimum of any scrambled cost function by continuous time Hamiltonian evolution. The quantum adiabatic algorithm is only a special case of continuous time Hamiltonian evolution. The theorem says that for a totally unstructured, i.e scrambled, cost function no quantum algorithm can achieve more than Grover speed up.

Scrambled Theorem (modified from [5]). *Let $h(z)$ be a cost function, with $h(0) = 0$ and $h(1), h(2), ..., h(N-1)$ all positive. Let π be a permutation on N elements, and $H_D(t)$ be an arbitrary π-independent Hamiltonian. Consider the Hamiltonian*

$$\tilde{H}_\pi(t) = H_D(t) + c(t)\left(\sum_{z=0}^{N-1} h(\pi^{-1}(z))|z\rangle\langle z|\right),$$

where $|c(t)| \leq 1$ *for all* t. *Let* $|\psi_\pi(T)\rangle$ *be the state obtained by Schrodinger evolution governed by* $\tilde{H}_\pi(t)$ *for time* T, *with a* π*-independent starting state. Suppose that the success probability* $|\langle\psi_\pi(T)|\pi(0)\rangle|^2 \geq \frac{1}{2}$, *for a set of* $\epsilon N!$ *permutations. Then*

$$T \;\geq\; \frac{\epsilon^2\sqrt{N}}{64h^\star} \;\; \textit{for } N \geq \frac{256}{\epsilon}.$$

where

$$h^\star = \left(\frac{\sum_z h(z)^2}{N-1}\right)^{\frac{1}{2}}.$$

We now return to the quantum adiabatic Hamiltonian $H_\pi(s)$ given by (3) and apply the Adiabatic Theorem. We have

$$\gamma_\pi(0) = \gamma_\pi(1) = 1$$

and

$$\left\|\frac{dH}{ds}\right\| \leq 2n.$$

Here $N = 2^n$. Furthermore the ground state at $s = 1$ is $|\phi(1)\rangle = |\pi(0)\rangle$. The state $|\psi_\pi(T)\rangle$ is obtained by evolving with the Hamiltonian $H_\pi\left(\frac{t}{T}\right)$ starting from the state $|x = 0\rangle$. Plugging into the Adiabatic Theorem we get

$$\begin{aligned}\sqrt{\left(1 - |\langle\psi_\pi(T)|\pi(0)\rangle|^2\right)} \;&\leq\; \frac{1}{T}\left[4n + \int_0^1 \frac{28n^2}{\gamma_\pi^3} ds\right] \\ &\leq\; \frac{1}{T}\left[4n + \frac{28n^2}{g_\pi^3}\right] \\ &\leq\; \frac{32n^2}{Tg_\pi^3} \end{aligned} \tag{9}$$

where in the last line we used the fact that $g_\pi \leq \gamma_\pi(0) = 1$.

Fix $0 < \epsilon < 1$. Let R be the set of permutations π for which

$$g_\pi > \left(\frac{32n^3}{\left[\frac{\epsilon^2}{128}\sqrt{N}\right]}\right)^{\frac{1}{3}}. \tag{10}$$

Then plugging into (9) we get

$$\sqrt{\left(1 - |\langle\psi_\pi(T)|\pi(0)\rangle|^2\right)} \leq \frac{\left(\frac{\epsilon^2}{128n}\sqrt{N}\right)}{T} \text{ for all } \pi \in R.$$

Now choose

$$T = \frac{\sqrt{2}\epsilon^2}{128n}\sqrt{N} \tag{11}$$

which guarantees that $|\langle\psi_\pi(T)|\pi(0)\rangle|^2 \geq \frac{1}{2}$ for all $\pi \in R$. Assume (to get a contradiction) that the size of R is at least $\epsilon N!$. Now apply the Scrambled Theorem to obtain (for $N \geq \frac{256}{\epsilon}$)

$$T \;\geq\; \frac{\epsilon^2}{64n}\sqrt{N}$$

where we have used the fact that in our case $h^\star \leq n$. But (11) contradicts the last inequality. Therefore R cannot contain $\epsilon N!$ permutations when N is sufficiently large. In other words, for $N \geq \frac{256}{\epsilon}$

$$\Pr\left[g_\pi \leq \left(\frac{32n^3}{\left\lceil\frac{\epsilon^2}{128}\sqrt{N}\right\rceil}\right)^{\frac{1}{3}}\right] \geq 1-\epsilon.$$

For example choosing $\epsilon = \frac{64}{n\sqrt{n}}$ we get Theorem 2 in the stated form.

D. Proof of Theorem 3

For any Hamiltonian H, the first excited state energy E_1 is equal to

$$E_1 = \max_{|\phi\rangle}\left[\min_{|\psi\rangle \text{ s.t } \langle\phi|\psi\rangle=0} \langle\psi|H|\psi\rangle\right]$$

where $\langle\psi|\psi\rangle = 1$. Let us now apply this fact to bound the first excited state energy $E_{1,\pi}(s)$ of $H_\pi(s)$. We can get a lower bound on $E_{1,\pi}(s)$ by fixing $|\phi\rangle$ to be a particular state. Choosing $|\phi\rangle = |\pi(0)\rangle$ gives

$$E_{1,\pi}(s) \geq \min_{|\psi\rangle \text{ s.t } \langle\pi(0)|\psi\rangle=0} \langle\psi|H_\pi(s)|\psi\rangle.$$

Now the quantity on the RHS is the ground state energy of the Hamiltonian obtained from $H_\pi(s)$ by removing one row and one column corresponding to the state $|\pi(0)\rangle$. This reduced Hamiltonian is stoquastic and applying Theorem 4 to it gives a lower bound

$$E_{1,\pi}(s) \geq \min_{z \neq \pi(0)} \frac{\langle z|H_\pi(s)|\chi\rangle}{\langle z|\chi\rangle} \tag{12}$$

for any state $|\chi\rangle$ such that $\langle y|\chi\rangle > 0$ for all bit strings $y \neq \pi(0)$ and $\langle\pi(0)|\chi\rangle = 0$.

We will use the bound (12) with a state $|\chi_\pi\rangle$ defined by

$$\langle z|\chi_\pi\rangle = \begin{cases} 1 & , \; z \notin \tilde{S}_\pi \\ \mu n & , \; z \in \tilde{S}_\pi \\ 0 & , \; z = \pi(0). \end{cases}$$

where μ depending on s will be chosen later and

$$\tilde{S}_\pi = \left\{ z : \; z \neq \pi(0) \text{ and } W(\pi^{-1}(z)) \leq nc \right\}$$

for some c which we will also choose later. $\tilde{S}_\pi$ is the image of the set $\{z : \; z \neq 0 \text{ and } W(z) \leq nc\}$ under the permutation π. For n large enough we will have $\mu n \geq 1$.

To evaluate the RHS of (12) we need

$$\begin{aligned}
\frac{\langle z|H_\pi(s)|\chi_\pi\rangle}{\langle z|\chi_\pi\rangle} &= sW\left(\pi^{-1}(z)\right) + \left(\frac{1-s}{2}\right) n - \left(\frac{1-s}{2}\right) \sum_{i=1}^{n} \frac{\langle z \oplus e_i|\chi_\pi\rangle}{\langle z|\chi_\pi\rangle} \\
&\geq \begin{cases} s + \left(\frac{1-s}{2}\right) n - \left(\frac{1-s}{2}\right) \sum_{i=1}^{n} \frac{\langle z \oplus e_i|\chi_\pi\rangle}{\langle z|\chi_\pi\rangle} & , \text{ for } z \in \tilde{S}_\pi \\ s \cdot nc + \left(\frac{1-s}{2}\right) n - \left(\frac{1-s}{2}\right) \sum_{i=1}^{n} \frac{\langle z \oplus e_i|\chi_\pi\rangle}{\langle z|\chi_\pi\rangle} & , \text{ for } z \notin \tilde{S}_\pi \text{ and } z \neq \pi(0). \end{cases}
\end{aligned}$$

The set $\tilde{S}_\pi$ has cardinality

$$\left|\tilde{S}_\pi\right| \leq 2^{f(c)n}$$

where $f(x)$ is given by (7). Applying Lemma 2 with $k = 2$ we get that with probability at least $1 - n^2 \cdot 2^{n[1-2(1-f(c))]}$ there is no pair of one bit flip neighbors

$$\{z, z \oplus e_j\} \subseteq \tilde{S}_\pi$$

and similarly with probability at least $1 - n^2 \cdot 2^{n[1-2(1-f(c))]}$ there is no set

$$\{z \oplus e_{j_1}, z \oplus e_{j_2}\} \subseteq \tilde{S}_\pi.$$

Choose $c < \frac{1}{2}$ to make $f(c) = 0.49$. Then with probability at least $1 - 2n^2 2^{-0.02n}$ we have

$$\begin{aligned}
\frac{\langle z|H_\pi(s)|\chi_\pi\rangle}{\langle z|\chi_\pi\rangle} &\geq \begin{cases} s + \left(\frac{1-s}{2}\right) n - \left(\frac{1-s}{2}\right) \frac{1}{\mu} & , \text{ for } z \in \tilde{S}_\pi \\ s \cdot nc + \left(\frac{1-s}{2}\right) n - \left(\frac{1-s}{2}\right) [n\mu + n - 1] & , \text{ for } z \notin \tilde{S}_\pi \, , \, z \neq \pi(0) \end{cases} \\
&= \begin{cases} \left(\frac{1-s}{2}\right) n - \left(\frac{1-s}{2}\right) \left[\frac{1}{\mu} - \frac{2s}{1-s}\right] & , \text{ for } z \in \tilde{S}_\pi \\ \left(\frac{1-s}{2}\right) n - \left(\frac{1-s}{2}\right) \left[n\left(\mu + 1\right) - 1 - \frac{2snc}{1-s}\right] & , \text{ for } z \notin \tilde{S}_\pi \, , \, z \neq \pi(0). \end{cases}
\end{aligned} \tag{13}$$

For $s > \frac{1}{1+2c} \approx 0.82$ choose μ to be

$$\mu = \frac{2sc}{1-s} - 1.$$

Then

$$\left(\frac{1-s}{2}\right) \left[n\left(\mu + 1\right) - 1 - \frac{2snc}{1-s}\right] = -\left(\frac{1-s}{2}\right)$$

and

$$\left(\frac{1-s}{2}\right)\left[\frac{1}{\mu}-\frac{2s}{1-s}\right] \;=\; \frac{1-s^2\,(1+4c)}{2s\,(1+2c)-2}. \tag{14}$$

Plugging this into (13) gives that with probability at least $1-n^2 2^{-0.02n}$, for $0.9 \leq s \leq 1$,

$$E_{1,\pi}(s) \geq \min_{z\neq\pi(0)} \frac{\langle z|H_\pi(s)|\chi_\pi\rangle}{\langle z|\chi_\pi\rangle} \geq \left(\frac{1-s}{2}\right) n + \frac{s^2\,(1+4c)-1}{2s\,(1+2c)-2}.$$

Then since the ground state energy of $H_\pi(s)$ is less than or equal to $\left(\frac{1-s}{2}\right) n$, the gap is bounded below by the second term on the RHS, with probability at least $1-n^2 2^{-0.02n}$. For $0.9 \leq s \leq 1$ this term is larger than 0.8. This completes the proof.

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